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Atomistic Simulation of Point Defects and Dislocations in bcc Transition Metals from First Principles*

Wei Xu and John A. Moriarty
Lawrence Livermore National Laboratory
University of California
Livermore, CA 94551

Multi-scale modeling of mechanical properties often requires an accurate atomistic description of defect energetics as input to larger length-scale theories. Using multi-ion interatomic potentials derived from first-principles generalized pseudopotential theory [1], we are studying point defects and dislocations in bcc transition metals, with molybdenum (Mo) as a prototype. Many-body angular forces, which are important for such central transition metals with partially filled *d* bands, are accounted for in the present theory through explicit three- and four-ion potentials. For point defects in Mo, the calculated vacancy formation and activation energies are in excellent agreement with experimental results. The energetics of six self-interstitial configurations in Mo have also been investigated. The <110> split dumb-bell interstitial is found to have the lowest formation energy, in agreement with the configuration found by X-ray diffuse scattering measurements. In ascending order, the sequence of energetically stable interstitials is: <110> split dumb- bell, tetrahedral site, crowdion, <111> split dumb-bell, <100> split dumb-bell, and octahedral site. In addition, the migration paths for the <110> dumb-bell self-interstitial in Mo have been studied. The migration energy is found to be one order of magnitude higher than previous theoretical estimates obtained using a simple radial-force Finnis-Sinclair potential for Mo [2,3]. Finally, the energetics and core structure of the <111> screw dislocation in Mo are being investigated, and the calculations are also being extended to tantalum. These results will be compared with available experimental data as well as the results of other theoretical studies.

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